

Advancements in the design and validation of an air pollution integrated assessment model for Spain

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ABSTRACT

This paper describes the design and application of the Atmospheric Evaluation and Research Integrated model for Spain (AERIS). Currently, AERIS can provide concentration profiles of NO₂, O₃, SO₂, NH₃, PM, as a response to emission variations of relevant sectors in Spain. Results are calculated using transfer matrices based on an air quality modelling system (AQMS) composed by the WRF (meteorology), SMOKE (emissions) and CMAQ (atmospheric-chemical processes) models. The AERIS outputs were statistically tested against the conventional AQMS and observations, revealing a good agreement in both cases. At the moment, integrated assessment in AERIS focuses only on the link between emissions and concentrations. The quantification of deposition, impacts (health, ecosystems) and costs will be introduced in the future. In conclusion, the main asset of AERIS is its accuracy in predicting air quality outcomes for different scenarios through a simple yet robust modelling framework, avoiding complex programming and long computing times.

Keywords:

Integrated Assessment Model
Air quality modelling
Iberian Peninsula
Decision support
Air pollution

Software availability

Name of Software: AERIS
Developer: Michel Vedrenne

Year first available: 2013
Hardware required: PC Compatible
Software required: Windows®, MATLAB® 7.10
Program language: C/C++, Java 1.6
Program size: 31 MB
Availability and cost: Contact developer. m.vedrenne@upm.es

Abbreviations: AERIS, Atmospheric Evaluation and Research Integrated model for Spain; AOT₄₀, Accumulated dose over a threshold of 40 ppb of ozone; AQMS, Air Quality Modelling System; BAT, Best available technique; BS, Baseline scenario (2007); CB, Carbon Bond mechanism; CMAQ, Community Multiscale Air Quality model; CPU, Central Processing Unit; E, Emissions; ECMWF, European Centre for Medium Range Weather Forecasts; EMEP, European Monitoring and Evaluation Programme; FAC2, Factor of two; GAINS, Greenhouse Gas and Air Pollution Interactions and Synergies model; GUI, Graphic User Interface; HS, Hypothetic scenario; IA, Integrated Assessment; IAM, Integrated Assessment Model; MB, Mean Bias; ME, Mean Error; NMB, Normalized Mean Bias; NME, Normalized Mean Error; PC, Personal Computer; PM, Particulate Matter; PNEI, National Emission Inventory of Portugal; PR, Projected Emissions; RAINS, Regional Air Pollution and Simulation model; RS₁₁, Real emission scenario for year 2011; RS₁₄, Real emission scenario for year 2014; S, Sector; SEP, Spain's Emission Projections model; SERCA, Sistema de Evaluación de Riesgos por Contaminación Atmosférica en la península Ibérica; SIMCA, Sistema Integrado de Modelización de la Contaminación Atmosférica; SMOKE, Sparse Matrix Operator Kernel Emissions model; SNAP, Selected Nomenclature for Air Pollution; SNEI, National Emission Inventory of Spain; SOMO₃₅, Sum over means of 35 ppb of ozone; TM, Transfer Matrix; UNECE, United Nations Economic Commission for Europe; USGS, United States Geological Survey; VP, Variation Percentage; WRF, Weather Research and Forecast model.

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1. Introduction

Integrated Assessment (IA) models are tools aimed to describe quantitatively the cause–effect relationship of events, cross-linkages and connections between issues of a given problem, seeking to analyse it under a synoptic perspective (Alcamo et al., 2002). These models provide a comprehensive framework for a shared and focused understanding of environmental challenges and have been applied to different sectors under various perspective. To this respect, issues such as climate change, air pollution, water management or environmental security are currently being addressed under integrated assessment approaches (de Vos et al., 2013; Kelly (Letcher) et al., 2013).

In line with the abovementioned, modelling air pollution under an IA approach is appropriate since the entire phenomenon is a consequence of complex interactions between physical and human systems. Typically, air pollution IA models (IAMs) describe the links between the emissions of pollutants, their atmospheric transport and chemical transformations, as well as the

environmental and health impacts they produce (Carnevale et al., 2012). In other words, air pollution IAMs cover the complete chain of events that links human activities (emissions) to environmental effects that can ultimately be translated into economic losses (impacts).

The use of IAMs as policy-support tools in Europe has become common in the recent decades as a consequence of the application of the UNECE Convention on Long Range Transboundary Air Pollution (CLRTAP) (Kaldellis et al., 2007). Examples of these are the Abatement Strategies Assessment Model (ASAM) (Warren and ApSimon, 1999) and the RAINS/GAINS Integrated Assessment system (Schöpp et al., 1999; Amann et al., 2011). While RAINS/GAINS is the most widely-used IAM for policymaking and negotiations at the European level, the need of operative IAMs at the national level has originated country-specific adaptations such as the GAINS-Italy (Vialeto et al., 2005; D'Elia et al., 2009), RAINS-NL (Aben et al., 2008) or the IMP model from Ireland (Kelly, 2006). Other models such as the United Kingdom Integrated Assessment Model (UKIAM) (Oxley et al., 2003) or the MINNI model for Italy (Zanini et al., 2005) have been developed independently.

In the same line, the Technical University of Madrid (UPM) has developed AERIS (Atmospheric Evaluation and Research Integrated Model for Spain), an IAM especially suited for Spain and the Iberian Peninsula. AERIS was created to be a reliable tool for support needed by policymakers at local, regional and national levels, trying to be useful to as many stakeholders as possible. This is especially relevant for Spain, whose institutional division in 17 autonomous communities makes necessary the elaboration of different regional air quality management plans. Furthermore, it should provide answers about whether the environmental objectives will be sufficiently met, as well as the associated economic and environmental consequences. An additional motivation for creating AERIS is the fact that continental IAMs are unable to deliver spatially resolved results suitable for national or regional policies and are usually restricted to Europe-wide common features, being national particularities out of reach (D'Elia et al., 2009). Furthermore, the ancillary information used for the compilation of emission inventories (i.e. bottom-up approaches) or the description of the meteorological conditions is usually of a better quality (Moussiopoulos et al., 2012).

The presented version of AERIS is able to estimate ambient concentrations produced by changes in the emissions of airborne pollutants. AERIS was built relying on the application of a robust air quality modelling system (AQMS), developed through the SIMCA and SERCA projects, which concentrate the experience accumulated over the years in emissions and air quality modelling. It should be noted that AERIS is intended to mimic comprehensive systems used for scenario analysis and policy support in Spain (Guevara et al., 2013; Borge et al., 2014) as well as air quality impact assessment (de Andrés et al., 2012; Boldo et al., 2014), but it cannot be used as a screening tool for air quality forecasting (Baldasano et al., 2008).

Furthermore, AERIS was been created to be simple and flexible without sacrificing the quality of the results. Its construction implied using country-specific data provided by national administrations, always working with a fine resolution ($16 \times 16 \text{ km}^2$) which is very necessary when allocating abatement measures (Oxley and ApSimon, 2007; Moussiopoulos et al., 2009). This resolution can be considered an intermediate step between the continental and the urban scales, which is appropriate for the multi-scalar nesting of models (Oxley et al., 2009). It is also worth noting that the quantification of emissions relied on the use of inventories which were constructed using data referred to the regional and local scales rather than European-scale estimates (i.e. EMEP).

This work describes in its first part the methodology followed in the modelling and construction process of AERIS. The second part is devoted to evaluating the performance of AERIS against two different emission scenarios by comparing its outputs to those of the standard AQMS as well as air quality observations. Finally a discussion on the relevance and robustness of the outputs produced by AERIS is carried out. In general lines, the objective of this paper is the description and validation of the current developments in the advancement of integrated assessment modelling to the air pollution problem in Spain by the means of AERIS.

In a more general perspective, this paper intends to present AERIS as an example of wider integrated assessment modelling and to provide relevant guidance on generic issues on problem areas encountered by modellers and stakeholders. Furthermore, the AERIS example should help fostering a more informed and creative decision-making environment and respond to the challenges to science practice with other stakeholders such as politics, governance, media, etc (Kelly (Letcher) et al., 2013). The ultimate objective is to favour openness in front of bodies of expertise that lie beyond the boundaries of formal science (Berkhout, 2010).

2. The AERIS model

2.1. General overview

The AERIS model is a multi-pollutant modular IAM that addresses air quality changes, expressed in terms of policy-relevant indicators, as a function of variations in the emissions. The relevant compounds described by AERIS are sulphur dioxide (SO_2), nitrogen oxides (NO_x), ammonia (NH_3), two fractions of particulate matter (PM_{10} , $\text{PM}_{2.5}$), and non-methane volatile organic compounds (VOC). The model also includes tropospheric ozone (O_3) and secondary particles. In general terms, AERIS has been created to take into consideration the emissions of each of the before mentioned primary pollutants in Spain and Portugal as well as their transport and transformation across the modelled domain. The results are presented as a series of air quality indicators derived from Directive 2008/50/EC on ambient air quality and cleaner air for Europe (EC, 2008). These indicators are linked to the possible impacts that air pollution has on human health, ecosystems, etc.

Table 1

List of policy-relevant air quality indicators considered by AERIS (Directive 2008/50/EC).

Pollutant	Indicators – (units)
NO_2	Mean monthly concentration – ($\mu\text{g}/\text{m}^3$)
	Mean annual concentration – ($\mu\text{g}/\text{m}^3$)
SO_2	19th highest hourly concentration – ($\mu\text{g}/\text{m}^3$) ^a
	Mean monthly concentration – ($\mu\text{g}/\text{m}^3$)
	Mean annual concentration – ($\mu\text{g}/\text{m}^3$)
	25th highest hourly concentration – ($\mu\text{g}/\text{m}^3$) ^a
NH_3	4th highest daily concentration – ($\mu\text{g}/\text{m}^3$) ^a
	Mean monthly concentration – ($\mu\text{g}/\text{m}^3$)
PM_{10}	Mean annual concentration – ($\mu\text{g}/\text{m}^3$)
	Mean monthly concentration – ($\mu\text{g}/\text{m}^3$)
$\text{PM}_{2.5}$	Mean annual concentration – ($\mu\text{g}/\text{m}^3$)
	36th highest daily concentration – ($\mu\text{g}/\text{m}^3$) ^a
O_3	Mean monthly concentration – ($\mu\text{g}/\text{m}^3$)
	Mean annual concentration – ($\mu\text{g}/\text{m}^3$)
	26th highest maximum daily 8-h value – ($\mu\text{g}/\text{m}^3$) ^a
	Sum of means over 35 ppb (SOMO_{35}) – ($\mu\text{g}/\text{m}^3 \text{ h}$)
	Daylight accumulated dose over a threshold of 40 ppb (AOT_{40}) – ($\mu\text{g}/\text{m}^3 \text{ h}$) ^a

^a Indicators derived from Directive 2008/50/EC to define limit values, target values or critical levels.

and are presented in Table 1. Presently only ambient air concentration levels are addressed, but in future versions of AERIS, these indicators will be linked to health impacts, as well as suited for a closer integration and linkage with European-scale IAMs in order to develop the costs and optimization modules.

The domain described by AERIS consists of a grid of 4550 cells of 16×16 km, arranged in a grid of 75×60 ($m \times n$) cells centred in 40°N and 3°W which covers the entire Iberian Peninsula, and the Balearic Islands as well as Andorra, parts of France, Morocco and Algeria (Fig. 1). The election of the resolution is usually a result of the compromise between an assumable computational cost (in terms of the hardware infrastructure), the availability of data and their representativeness at that scale. Additionally, analysis at this scale is able to describe approximately emission abatement strategies and air quality changes relevant at mesoscale.

The structure of the current version of the AERIS model is modular, following the current trends in IA modelling. Since IAMs should consider all the interacting processes involved, the segmentation of AERIS in modules is advantageous when bringing together expertise from various disciplines (i.e. describing health impacts or monetary evaluations) (Hinkel, 2009). The following sections describe in detail each of the modules comprised by AERIS (Fig. 2).

2.2. Emission module

The emission module of AERIS has been built considering emissions taken from the National Emission Inventories of Spain (SNEI) and Portugal (PNEI) (MARM, 2009; APA, 2010) as well as EMEP gridded-emissions for the rest of the countries (Andorra, France, Morocco and Algeria). The emission inventories of Spain and Portugal are mixed-approach inventories (top-down and bottom-up) while the EMEP gridded-emissions are compiled using

estimates reported by the respective national authorities. A major effort was made to harmonize as much as possible the national inventories from Portugal and Spain, while the emissions from large point-source were individually managed following the methodology published in Borge et al. (2008a). The annual emissions reported in the before mentioned inventories were processed using the SMOKE model in order to prepare hourly-gridded data for air quality simulations (IE, 2009). The chemical speciation, temporal and spatial allocation procedures as well as the complete configuration of the SMOKE model to the Iberian conditions was carried out according to Borge et al. (2008a). This included emissions from 184 area-source and 62 point-source categories for Spain and Portugal, as well as international maritime activities configured as explained in Section 2.3 (Borge et al., 2014).

It is important to indicate that AERIS is not able to calculate air quality levels from arbitrary emission data. In every case, consultations must be linked to a reference or baseline scenario (BS). The inclusion of a baseline scenario in AERIS constitutes an effective device to assess the robustness of environmental policies under different future conditions (Alcamo, 2008; Moussiopoulos et al., 2012).

Emissions (E) in the BS refer to the year 2007, which corresponds to a representative year of high economic growth and intense polluting activity in Spain, being the last year before the introduction of composition limits to fuels (MAGRAMA, 2013). Ideally, any abatement applied or agreed under new protocols will produce reductions in this baseline scenario. The BS encompasses a set of policy-relevant activities that are described under the SNAP nomenclature, according to the EMEP/CORINAIR methodology used in SNEI and PNEI (EEA, 2007). To this respect, AERIS considers the emissions of 18 sectors (some of which actually correspond to macrosectors) that were chosen by taking two factors into account: (i) the magnitude of their contribution to the

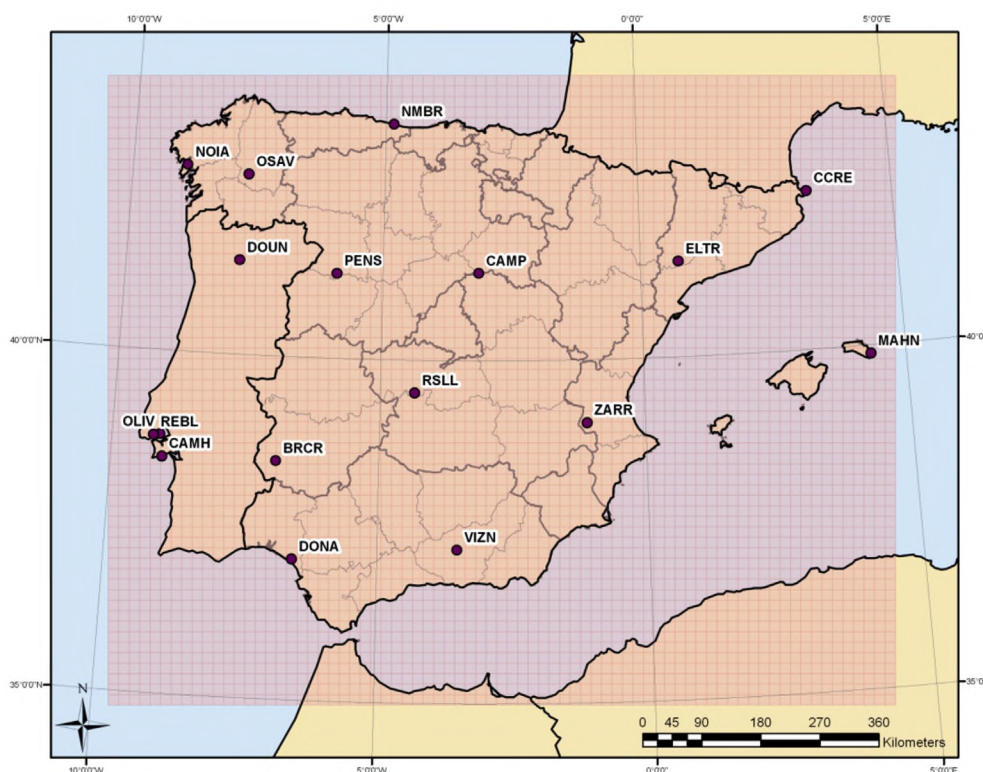


Fig. 1. Geographic representation of the modelled domain and monitoring locations used for validation (light red: domain considered by AERIS). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

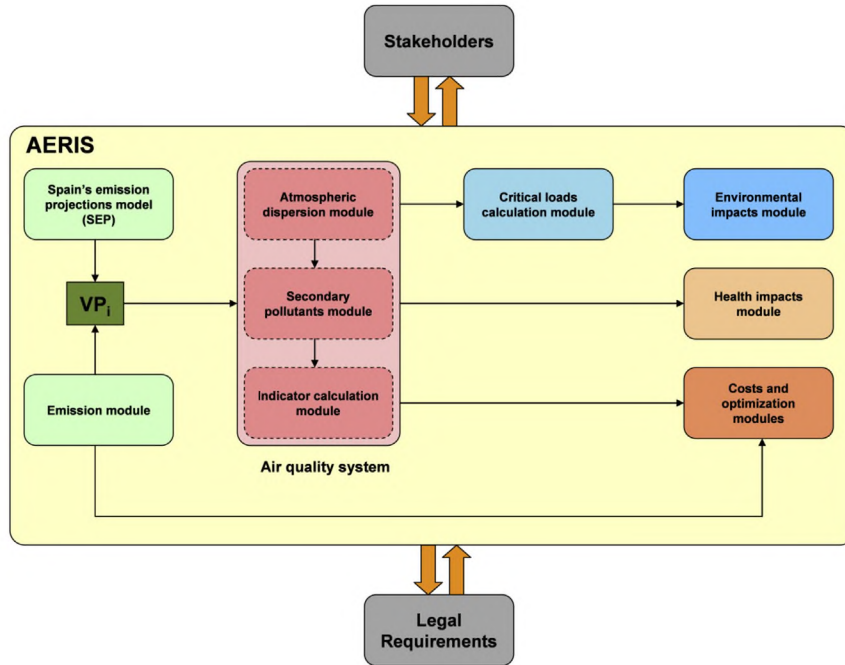


Fig. 2. Schematic flowchart of the AERIS modelling system. VP_i (green block) is the emissions variation percentage of sector i with respect to BS (see Section 2.2). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

total emissions in Spain and (ii) their susceptibility of being of interest for policy-regulation. Table 2 presents the emissions and contributions to the national total for the individual sectors at the BS (excluding Portugal). The relevance of the 18 considered sectors is evidenced by the total emissions and contributions listed at the end of Table 2.

The projected emissions of any emission sector for a given scenario can be computed with the Spain's Emission Projections Model (SEP), whose outputs are compatible with AERIS (Lumbreras et al., 2008) and which has been applied for a number of scenarios as published in Lumbreras et al. (2009). Focussing on a relevant sector (i), the projected emissions quantified by SEP ($PR_{i,i}$) allow the emission module to compare them with those of the baseline scenario ($BS_{i,i}$) and to consistently estimate a variation percentage (VP_i) as indicated in Eq. (1).

$$VP_i = 100 \cdot (E_{PR,i} - E_{BS,i}) / E_{BS,i} \quad (1)$$

The set of variation percentages that result from a hypothetical scenario (in which the emissions of several sectors might suffer changes) are necessary parameters to calculate the concentration of pollutants in the modelled domain with the atmospheric dispersion module. Moreover, applying a VP instead of absolute emissions allows considering another BS without altering the rest of the modules of AERIS. Any reductions in emissions were considered to be uniform across sectors. It should be noted that the algorithm of AERIS requires that the different VPs are provided by the user as a requisite to execute the atmospheric dispersion module.

2.3. Air quality system

The air quality system of AERIS describes the complex meteorological and chemical processes that influence air quality through the use of three sequential modules: atmospheric dispersion, secondary pollutants module and indicator calculation. Although differentiated, these three modules have been gathered to constitute the air quality system under a global idea of “atmospheric

transport and transformation module” (Fig. 2). In general, this system links changes in pollutants emissions at the various sources (quantified through a VP_i) to responses in impact-relevant air quality indicators for each of the modelled cells (Amann et al., 2011). Usually atmospheric dispersion modules rely on reduced-form representations of full AQMSs. To this respect, AERIS mimics air quality simulations based on the WRF model for the description of meteorology and the CMAQ model for the atmospheric chemistry and dispersion.

WRF is a mesoscale model that includes the latest developments for meteorological modelling under a fully compressible, non-hydrostatic approach (Skamarock and Klemp, 2008). The model inputs (terrain elevation, land use and land-water masks, soil humidity and temperatures) were obtained from USGS (Wickham et al., 2013) and the ECMWF (Isaksen et al., 2011). Further details on the dynamic options and parameterizations for the particular conditions of the Iberian Peninsula can be found in Borge et al. (2008b).

CMAQ is a multi-pollutant, multi-scale Eulerian air quality model whose algorithms can handle atmospheric dispersion along with the major issues concerning photochemical oxidants, particulate matter, and acidic and nutrient deposition under different reaction mechanisms (Byun and Schere, 2006). CMAQ was fed with emissions from the inventories mentioned in Section 2.2, which were chemically speciated according to the CB05 mechanism (Yarwood et al., 2005). In every experiment, chemical speciation profiles for NO_x , $PM_{2.5}$ and VOC were kept constant in every simulation. Finally, time-dependent boundary conditions were obtained from a larger domain at European-scale into which the modelled domain is nested (Borge et al., 2014).

The before mentioned AQMS allowed constructing a series of functional relationships for each of the activities considered in the BS (Table 2) through the use of transfer matrices (TM). Transfer matrices are sector and pollutant specific across the studied domain which means that there is one individual TM for every sector and pollutant that is considered by AERIS. In total, AERIS has 51 individual TMs of which 14 describe the emission-concentration

Table 2

Considered activities in AERIS. Emissions and National contributions (Spain) for the baseline scenario (BS)-2007.

SNAP code ^a	Activity name	NO _x ^b		SO ₂		PM ₁₀		PM _{2.5}		NH ₃	
010000	Coal-fired power plants >300 MW	235331	14.5%	805700	67.8%	17632	4.7%	14899	11.3%	98	<1%
020202	Residential plants <50 MW	19215	1.4%	12426	1.1%	23280	6.2%	21978	16.7%	0	0%
030000	Combustion in manufact.-area sources	197064	13.9%	63686	5.8%	8609	2.3%	6270	4.8%	0	0%
040000	Production processes-area sources	3958	<1%	33731	3.1%	7203	1.9%	3801	2.9%	14264	9.1%
070101	Passenger cars-Highway driving	124764	8.9%	558	<1%	4955	1.3%	4955	3.8%	5010	3.2%
070103	Passenger cars-Urban driving	65926	4.7%	506	<1%	7393	2.0%	7393	5.6%	246	<1%
070201	LDV < 3.5-Highway driving	19626	1.4%	145	<1%	1910	0.5%	1910	1.5%	107	<1%
070203	LDV < 3.5-Urban driving	39633	2.8%	224	<1%	3048	0.8%	3048	2.3%	37	<1%
070301	HDV > 3.5 t-Highway driving	100968	7.2%	500	<1%	3867	1.0%	3867	2.9%	76	<1%
070303	HDV > 3.5 t-Urban driving	56689	4.0%	226	<1%	2781	0.7%	2781	2.1%	28	<1%
0707 + 08	Break, tire and road abrasion processes	0	0%	0	0%	11,532	3.1%	6350	4.8%	0	0%
080500	Airports LTO/yr > 10.000	7310	<1%	343	<1%	9	<1%	9	<1%	0	0%
080600	Agriculture (machinery)	109898	7.8%	7865	0.8%	28727	16.9%	28727	21.9%	13	<1%
080800	Industry (machinery)	64913	4.6%	132	<1%	13761	8.1%	13761	10.5%	8	<1%
100101	Culture with fertilizers-permanent crops	3155	<1%	0	0%	0	0%	0	0%	91748	8.7%
100102	Culture with fertilizers-arable crops	8297	<1%	0	0%	730	<1%	0	0%	35218	22.5%
100500	Other agricultural activities	0	0%	0	0%	16553	8.7%	2825	1.9%	120639	29.6%
110000 ^b	Other sources and sinks	37093	2.6%	388	<1%	93	<1%	0	0%	100559	24.7%
—	Portugal (total)	145,250	—	22,918	—	80,563	—	64,762	—	48,970	—
—	Internacional ship transit	642,166	—	444,069	—	53,989	—	48,590	—	36	—
—	Total of Sectors^c	1093840	75.8%	926,430	77.9%	152,083	89.5%	122,574	92.9%	368,051	90.4%

^a Sectors 010000, 030000, 040000, 0707+08 and 110000 correspond to macrosectors.^b Emissions are presented in annual metric tons (t yr⁻¹).^c Excluding Portugal and International ship transit.

link for NO_x, 8 describe SO₂, 12 describe PM₁₀ and PM_{2.5} respectively and 5 describe NH₃. Table 3 presents the current availability of TMs by pollutant and considered sectors.

In general lines, TMs were generated by systematically perturbing emissions of one or more pollutants by a given percentage, re-running the AQMS and comparing the results with the reference or baseline scenario (Tarrasón et al., 2004) following the methodology published in Bartincki (1999) and Amann et al. (2011). For the construction of each TM, five annual runs were carried out by changing the emissions of the given sector around the 2007 baseline scenario (BS) with the following variation percentages: -90%, -50%, 0%, 50%, and 90% and statistically processing the concentration outputs. These percentages were chosen with the objective of covering the widest possible range of emission variations, and by paying special

attention to the maximum technically-feasible reductions for the relevant sectors (Amann et al., 2007). The use of positive and negative variations with the same absolute value (-90%/90%, -50%/50%) was made in order to minimize the nonlinearity effects of the advection algorithm according to what is discussed in Bott (1989). Due to limitations in hardware resources, TMs were built from experimental runs using the meteorology of year 2007 (BS) and thus assuming that the meteorology of this year is representative of future situations. It is worth noting that obtaining a TM is a complex and computer-intensive process, being this an additional motivation for considering only those sectors that accounted for the greatest emissions of a given pollutant (Table 3). Due to computing limitations and to the sector and pollutant-specific nature of TMs, conducting the parameterization with only five simulations was deemed sufficient for guaranteeing statistical consistence without compromising the laboratory's computing capacity. This fact is particularly true since it was observed that increasing the number of simulations for the construction of TMs slightly increased the quality of the statistical regression (Vedrenne et al., 2013). Additionally, it should be kept in mind that a TM is a statistical parameterization of model performance so limitations in the robustness of AERIS diagnostic capabilities should definitely be expected when compared to a deterministic AQMS.

2.3.1. Nitrogen dioxide (NO₂), sulphur dioxide (SO₂) and ammonia (NH₃)

The TMs prepared for NO₂, SO₂ and NH₃ allow calculating both, mean monthly and mean annual concentrations from percentual variations in emissions for every activity. Additionally, the 19th highest hourly concentration for NO₂ as well as the 25th highest hourly concentration and the 4th highest daily concentration for SO₂ can be computed (Table 1). Eqs. (2–4) represents the expressions for calculating indicators for NO₂, SO₂ and NH₃ respectively.

$$[\text{NO}_2]_{m \times n} = [k_{\text{indicator}, \text{NO}_2}]_{m \times n} \cdot \left(\sum_i \text{VP}_{\text{NO}_x, i} \cdot [\text{G}_{\text{NO}_x, i}]_{m \times n} + [\text{NO}_{2, \text{BS}}]_{m \times n} \right) \quad (2)$$

^a Bullets indicate that an individual transfer matrix (TM) is available.**Table 3**

Current availability of emission-concentration transfer matrices (TMs) in AERIS.

SNAP code	Activity name	NO ₂	SO ₂	PM ₁₀	PM _{2.5}	NH ₃
010000	Coal-fired power plants >300 MW	● ^a	●			
020202	Residential plants <50 MW	●	●	●	●	
030000	Combustion in manufact.-area sources	●	●			
040000	Production processes-area sources		●			
070101	Passenger cars-Highway driving	●		●	●	
070103	Passenger cars-Urban driving	●		●	●	
070201	LDV < 3.5-Highway driving	●		●	●	
070203	LDV < 3.5-Urban driving	●		●	●	
070301	HDV > 3.5 t-Highway driving	●		●	●	
070303	HDV > 3.5 t-Urban driving	●		●	●	
0707 + 08	Break, tire and road abrasion processes			●	●	
080500	Airports LTO/yr > 10,000	●				
080600	Agriculture (machinery)	●	●	●	●	
080800	Industry (machinery)	●	●	●	●	
100101	Culture with fertilizers-permanent crops					●
100102	Culture with fertilizers-arable crops					●
100500	Other agricultural activities			●	●	●
110000	Other sources and sinks					●
—	Portugal (total)	●	●	●	●	●
—	Internacional ship transit	●	●			

$$[\text{SO}_2]_{m \times n} = [k_{\text{indicator}, \text{SO}_2}]_{m \times n} \cdot \left(\sum_i \text{VP}_{\text{SO}_2, i} \cdot [\text{G}_{\text{SO}_2, i}]_{m \times n} + [\text{SO}_2, \text{BS}]_{m \times n} \right) \quad (3)$$

$$[\text{NH}_3]_{m \times n} = [k_{\text{indicator}, \text{NH}_3}]_{m \times n} \cdot \left(\sum_i \text{VP}_{\text{NH}_3, i} \cdot [\text{G}_{\text{NH}_3, i}]_{m \times n} + [\text{NH}_3, \text{BS}]_{m \times n} \right) \quad (4)$$

where:

$[\text{NO}_2, \text{SO}_2, \text{NH}_3]_{m \times n}$ —Ambient concentration of nitrogen dioxide, sulphur dioxide or ammonia expressed as a policy-relevant indicator ($\mu\text{g}/\text{m}^3$) with dimensions $m \times n = 75 \times 60$.¹ Expressed as the average concentration in the 16-km cell volume.

$[k_{\text{indicator}, \text{NO}_2, \text{SO}_2, \text{NH}_3}]_{m \times n}$ —Indicator-specific transformation matrix.

$\text{VP}_{\text{NO}_x, \text{SO}_2, \text{NH}_3, i}$ —Variation percentage of the NO_x , SO_2 or NH_3 emissions of sector i against the BS.

$[\text{G}_{\text{NO}_2, \text{SO}_2, \text{NH}_3, i}]_{m \times n}$ —TM of NO_x , SO_2 or NH_3 emissions of sector i .

$[\text{NO}_2, \text{BS}, \text{SO}_2, \text{BS}, \text{NH}_3, \text{BS}]_{m \times n}$ —Concentration of nitrogen dioxide, sulphur dioxide or ammonia at the BS ($\mu\text{g}/\text{m}^3$).

From Eqs. (2–4), it can be seen that for analysing any emission reduction scenario, AERIS considers the sum of the contributions of the respective TMs of those sectors on which emission reductions have concentrated. Modelling air quality levels in such a way obviously constitutes a simplification (i.e. linearization) of the complex deterministic processes that are described by the AQMS and is very likely to be a limiting factor in the model's robustness. The analysis of these potential limitations is addressed in Section 3.

2.3.2. Particulate matter (PM_{10} , $\text{PM}_{2.5}$)

AERIS is able to calculate the mean monthly concentration, the mean annual concentration and the 36th highest daily concentration ($\mu\text{g}/\text{m}^3$) for PM_{10} . In the case of $\text{PM}_{2.5}$, AERIS only provides data on mean monthly concentrations and the mean annual concentration ($\mu\text{g}/\text{m}^3$) (Table 1). Due to the fact that the air quality levels of particles are also influenced by the emission of precursor gases (NO_x , SO_2 or NH_3), the TMs for both PM_{10} and $\text{PM}_{2.5}$ have been modelled considering the contributions of these pollutants to secondary particle formation. Eq. (5) allows calculating any of the indicators mentioned above as a function of changes in the emissions of particulate matter itself, NO_x , SO_2 and NH_3 :

Expressed as the average concentration in the 16-km cell volume.

$k_{\text{indicator}}$ —Indicator-specific transformation matrix.

$\text{VP}_{\text{PM}_{x, i}}$ —Variation percentage of the PM_x emissions of sector i against the BS.

$[\text{G}_{\text{PM}_{x, i}}]_{m \times n}$ —TM of PM_x emissions of sector i .

$\text{VP}_{\text{NO}_x, i}$ —Variation percentage of the NO_x emissions of sector i against the BS.

$[\text{G}_{\text{NO}_x} - \text{PM}_{x, i}]_{m \times n}$ —TM of NO_x contributions to PM_x of sector i .

$\text{VP}_{\text{SO}_2, i}$ —Variation percentage of the SO_2 emissions of sector i against the BS.

$[\text{G}_{\text{SO}_2} - \text{PM}_{x, i}]_{m \times n}$ —TM of SO_2 contributions to PM_x of sector i .

$\text{VP}_{\text{NH}_3, i}$ —Variation percentage of the NH_3 emissions of sector i against the BS.

$[\text{G}_{\text{NH}_3} - \text{PM}_{x, i}]_{m \times n}$ —TM of NH_3 contributions to PM_x of sector i .

$[\text{PM}_x, \text{BS}]_{m \times n}$ —Particulate matter concentration at the BS ($\mu\text{g}/\text{m}^3$).

It is worth noting that Eq. (5) is not able to quantify the total mass of particulate matter, basically because it deals only with anthropogenic emissions and excludes completely the contribution of natural sources as well as primary and secondary organic aerosols. The adequateness of this linear approach to model the complex physicochemical processes that describe the formation of particles has been found to perform well when only marginal changes in emissions around a reference point are considered (Amann et al., 2011; Vedrenne et al., 2013).

2.3.3. Tropospheric ozone formation (O_3)

Traditionally, O_3 is a difficult pollutant to deal with due to the fact that it is not emitted directly, but rather formed from emissions of other substance. Moreover, the emission-concentration response of O_3 presents important non-linearities, especially with respect to the emissions of NO_x (Rypdal et al., 2005; Amann et al., 2011). To deal with these issues, AERIS calculates O_3 through a non-linear conversion module that correlates the resulting NO_2 concentrations after measures (expressed as the annual mean concentration of NO_2 calculated with Eq. (2)) and the VOC emissions with the ambient O_3 concentration (Carnevale et al., 2007). The expression for estimating the concentrations of O_3 was adapted from Guariso et al. (2004) and verified with the use of a surface-regression tool in MATLAB® (sftool). The regression coefficients were calculated following a response surface methodology according to Chi et al. (2012). Its general form is shown in Eq. (6), which is subject to the results calculated with Eq. (7):

$$[\text{PM}_x]_{m \times n} = k_{\text{indicator}} \cdot \left[\sum_i \left(\text{VP}_{\text{PM}_{x, i}} \cdot [\text{G}_{\text{PM}_{x, i}}]_{m \times n} + \text{VP}_{\text{NO}_x, i} \cdot [\text{G}_{\text{NO}_x - \text{PM}_{x, i}}]_{m \times n} + \text{VP}_{\text{SO}_2, i} \cdot [\text{G}_{\text{SO}_2 - \text{PM}_{x, i}}]_{m \times n} + \text{VP}_{\text{NH}_3, i} \cdot [\text{G}_{\text{NH}_3 - \text{PM}_{x, i}}]_{m \times n} \right) + [\text{PM}_x, \text{BS}]_{m \times n} \right] \quad (5)$$

where:

$[\text{PM}_x]_{m \times n}$ —Ambient particulate matter (PM_{10} or $\text{PM}_{2.5}$) concentration expressed as a policy-relevant indicator ($\mu\text{g}/\text{m}^3$).

$$[\text{O}_3]_{m \times n} = k_{\text{indicator}} \cdot \left([\text{G}_{00}]_{m \times n} + [\text{G}_{10}]_{m \times n} \cdot [\text{NO}_2]^*_{m \times n} + [\text{G}_{01}]_{m \times n} \cdot \text{VP}_{\text{VOC}} + [\text{G}_{11}]_{m \times n} \cdot [\text{NO}_2]^*_{m \times n} \cdot \text{VP}_{\text{VOC}} + [\text{G}_{20}]_{m \times n} \cdot [\text{NO}_2]^2_{m \times n} \right) \quad (6)$$

¹ Unless stated otherwise, hereinafter the $m \times n$ subindex refers to a dimension of 75×60 cells.

$$\text{subject to: } [\text{NO}_2]_{m \times n}^* = k_{\text{Annual Mean, NO}_2} \cdot \left(\sum_i \text{VP}_{\text{NO}_{x,i}} \cdot [\text{G}_{\text{NO}_{x,i}}]_{m \times n} + [\text{NO}_{2,\text{BS}}]_{m \times n} \right) \quad (7)$$

where:

$[\text{O}_3]_{m \times n}$ - Ambient ozone concentration expressed as a policy-relevant indicator ($\mu\text{g}/\text{m}^3$). Expressed as the average concentration in the 16-km cell volume.

$k_{\text{indicator}}$ -Indicator-specific transformation matrix.

$[\text{G}_{00}, \text{G}_{01}, \dots, \text{G}_{20}]_{m \times n}$ -Non-linear coefficient matrices for the transformation of ozone precursors.

$[\text{NO}_2]_{m \times n}^*$ - Annual mean concentration of nitrogen dioxide ($\mu\text{g}/\text{m}^3$) computed as in Eq. (7).

VP_{VOC} -Total variation percentage of the VOC emissions in the entire modelled domain.

The O_3 module of AERIS allows quantifying mean monthly concentrations, mean annual concentrations, SOMO_{35} , daylight AOT_{40} and the 26th highest maximum daily 8-h concentration (Table 1).

2.4. Interface characteristics and layout

It is important to keep in mind that the final users of AERIS might not necessarily be high-skilled computer users and could be unfamiliar to air quality modelling. As a consequence, AERIS is being delivered embedded in a MATLAB®-based GUI as final product. Its basic computational structure is represented in Fig. 3. MATLAB® is a programming language that supports cell arrays to the definition of classes in object-oriented programming. It is equipped with all the essential constructs of a higher programming language at a moderate cost. Its use and learning involves little programming skills, while providing quickness in simulations and results retrieval (Ibrahim, 2011). Moreover, it is quite efficient in dealing with text tabular data and its results are compatible with typical desktop applications such as Microsoft Excel® and ArcGIS®.

As software, AERIS provides an open environment equipped with sophisticated visualization capabilities that allow creating maps with a high quality and interpretative value. To this respect, outputs can be obtained as indicator maps (visually) while data can be exported in tabular text files (.csv, .txt). The purpose of delivering AERIS as a GUI is facilitating input file preparation and output file display while simultaneously minimizing the involvement of the user with the code. The graphic environment of AERIS was kept as simple and intuitive as possible, asking opinions from stakeholders, policy-makers and students on critical design issues such as layout, simplicity of use or organization.

3. Model evaluation

In order to assure that the estimates provided by AERIS are reasonable, it is essential to carry out an analysis on its consistence and robustness as to evaluate its “fitness-for-purpose”. No universal consensus has been reached so far on good practices to evaluate model performance (Chemel et al., 2010; Alexandrov et al., 2011). Aiming to be as rigorous as possible, the evaluation was conducted for two relevant aspects as shown in detail in the following sections. First, the congruence of the modelling approach was examined through an additivity test where the outputs of the AQMS were used as reference for assessment purposes. Then, in order to check the accuracy of AERIS estimates, its performance was compared: (i) against air-quality observations for year 2011 and (ii) against the predictions of the AQMS for a future emission scenario in 2014. It is worth noting that the results of the AQMS have been already contrasted against observations independently (de la Paz et al., 2013).

3.1. Additivity test

The purpose of conducting an additivity test as part of the model evaluation procedures is to check whether the general formulation of the model (Eqs. (2)–(5)) is adequate enough for reproducing the outputs yielded by the ordinary AQMS. The so-called additivity

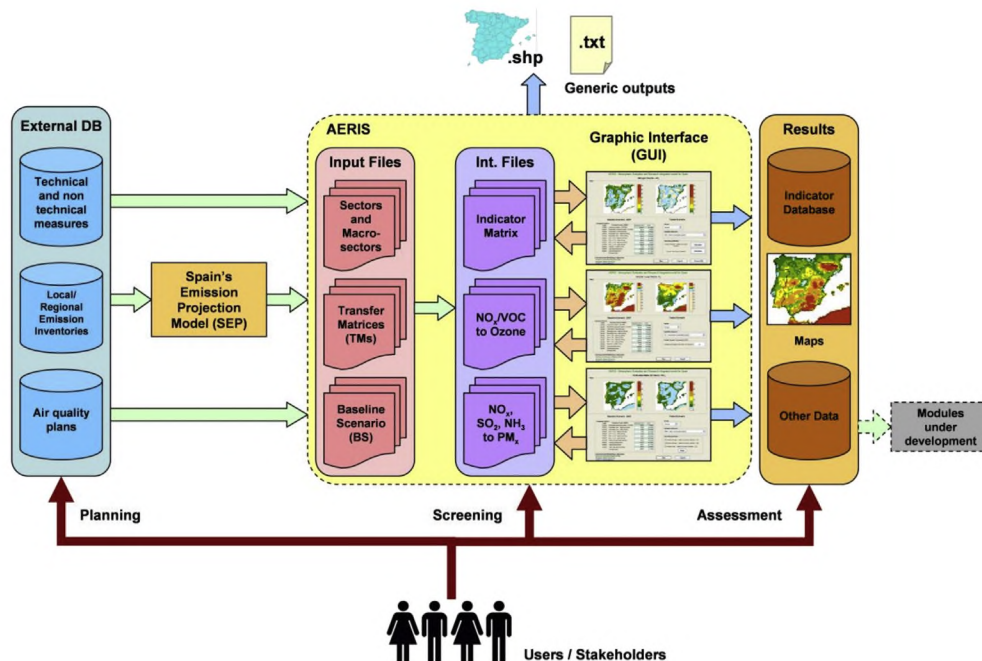


Fig. 3. Schematic flowchart of the structure and dependencies of AERIS.

Table 4
Selected monitoring locations for model validation.

Country	Station name	Code	X	Y	Measured pollutants
Spain	Barcarrota	BRCR	6°55'14"W	38°28'22"N	NO ₂ , O ₃ , SO ₂
Spain	Cabo de Creus	CCRE	3°18'56"E	42°19'09"N	NO ₂ , O ₃ , SO ₂
Spain	Campisábalos	CAMP	3°08'33"W	41°16'27"N	NO ₂ , O ₃ , SO ₂
Spain	Doñana	DONA	6°33'19"W	37°03'06"N	NO ₂ , O ₃ , SO ₂
Spain	Els Torms	ELTR	0°44'04"E	41°23'38"N	NO ₂ , O ₃ , SO ₂
Spain	Mahón	MAHN	4°19'26"E	39°52'33"N	NO ₂ , O ₃ , SO ₂
Spain	Niembro	NMBR	4°50'60"W	43°26'21"N	NO ₂ , O ₃ , SO ₂
Spain	Noia	NOIA	8°55'24"W	42°43'14"N	NO ₂ , O ₃ , SO ₂
Spain	O Saviñao	OSAV	7°42'16"W	42°38'14"N	NO ₂ , O ₃ , SO ₂
Spain	Peñausende	PENS	5°53'51"W	41°14'20"N	NO ₂ , O ₃ , SO ₂
Spain	Risco Llano	RSLL	4°21'11"W	39°31'15"N	NO ₂ , O ₃ , SO ₂
Spain	Viznar	VIZN	6°32'03"W	37°14'13"N	NO ₂ , O ₃ , SO ₂
Spain	Zarra	ZARR	1°06'03"W	39°04'58"N	NO ₂ , O ₃ , SO ₂
Portugal	Camarinha	CAMH	9°02'51"W	38°26'49"N	NO ₂ , O ₃ , SO ₂ , PM _{2.5}
Portugal	Douro Norte	DOUN	7°47'44"W	41°22'27"N	NO ₂ , O ₃ , SO ₂ , PM _{2.5}
Portugal	Olivais	OLIV	9°06'25"W	38°46'12"N	NO ₂ , O ₃ , SO ₂ , PM _{2.5}
Portugal	Reboleira	REBL	9°13'50"W	38°45'15"N	NO ₂ , O ₃ , SO ₂ , PM _{2.5}

constitutes a comparison between the total accumulation of error from simulations with sectors varying independently and the total error produced by a simulation in which the same sectors varied simultaneously. This test was applied with guidance from Schöpp et al. (2005) and Bennett et al. (2013). The analysis focused on NO₂ due to the fact that it is a primary pollutant that also participates in the complex interplay of particulate matter and O₃ formation, so an indirect picture of the general behaviour of the approach for other pollutants can be obtained. The rest of pollutants were not evaluated with the additivity test due to limitations in computing-time. The analysis was carried out by defining a simple hypothetical scenario (HS), with a definite number of sectors (S₁, S₂, ...S_N) whose NO_x emissions were varied. Each of these variations was processed separately with AERIS and the ordinary AQMS and their respective results compared. The HS was also simulated completely by both models and the obtained estimates compared. We assessed whether the following condition was fulfilled for three different thresholds (t) of 0.5, 1.0 and 1.5 µg/m³ (Eq. (8)):

$$\sum_i |S_{i, \text{AERIS}} - S_{i, \text{AQMS}}| - |HS_{\text{AERIS}} - HS_{\text{AQMS}}| \leq t \quad (8)$$

$$t = \{0.5, 1.0, 1.5 \text{ µg/m}^3\}$$

The lowest threshold ($t = 0.5 \text{ µg/m}^3$) was selected because it corresponds approximately to the mean absolute error of NO₂ predicted by AERIS (0.49 µg/m³) for a fully-described emission scenario evaluated in Vedrenne et al. (2013). The other thresholds are twofold and threefold this concentration value respectively. To this respect, we considered the approach is adequate enough in those cells below the first threshold, meaning that the accumulation of error due to the independent use of TMs is analogous to the error associated with the simultaneous use of TMs. Despite the fact

that AERIS is able to provide a variety of air quality indicators, the analysis was carried out using exclusively annual mean concentrations data.

3.2. General performance analysis of AERIS

The objective of this section is analysing through a concurrent comparison the general skills of AERIS while reproducing: (a) the predictions of the AQMS and (b) air-quality observations in order to justify its use while also aiming to recognize its limitations (Bennett et al., 2013). The validation rationale is based on model performance criteria according to Boylan and Russell (2006), USEPA (2007) and Chemel et al. (2010).

3.2.1. Validation of AERIS against AQMS

The results produced by AERIS have been contrasted against the predictions of the AQMS for a future emission scenario (2014). It is worth noting that the 2014-scenario included more sectors whose emissions varied than the actual number of sectors considered by AERIS (Table 3). As a result, some degree of deviation between the results produced by the AQMS and AERIS is to be expected. In a broader sense, this analysis should indicate about the suitability of AERIS as a screening tool whose results are comparable to those of the AQMS. Analysis focused on the annual mean concentrations of NO₂, SO₂, PM_{2.5}, NH₃ and O₃ produced by one year-run of AERIS and the AQMS respectively.

3.2.2. Validation of AERIS against observations

Modelled concentrations by AERIS were compared against measurements from the EMEP monitoring network (www.emep.int) located in Spain and Portugal for year 2011 (Table 4). The spatial coverage of the monitoring network is shown in Fig. 1, being composed only of rural background stations whose measurements are deemed representative of the spatial scale of AERIS (16 km). Although this methodology has little discriminating power to understand model behaviour, the objective of the validation practice is determining whether AERIS is able to replicate observed values. Comparisons were made exclusively for NO₂, O₃, PM_{2.5} and SO₂ and for the following relevant indicators: 19th highest hourly concentration (NO₂), daylight AOT₄₀ (O₃), mean annual concentration (PM_{2.5}) and 25th highest hourly concentration (SO₂).

3.2.3. Statistical metrics and diagrams

In the spirit of reducing the complexity of the evaluations, a series of statistical indicators was chosen in order to quantitatively characterize the performance. The most suitable indicators for model benchmarking and evaluation are residual indicators (Table 5) which calculate the difference between observed and modelled data pairs (Thunis et al., 2011; Bennett et al., 2013). Statistics were calculated separately for all species but values are given in a domain-wide basis. Scatter plots were used as diagnosis diagrams, evaluating in every case if data pairs distributed along a unity-slope line through the origin.

Table 5
Statistic indicators used for model comparisons and benchmarking.

Indicator	Definition	Units	Range
Mean Bias (MB)	$MB = \frac{1}{N} \cdot \sum_{i=1}^N (P_i - M_i)^a$	µg/m ³	−∞ – ∞
Mean Error (ME)	$ME = \frac{1}{N} \cdot \sum_{i=1}^N P_i - M_i $	µg/m ³	0 – ∞
Normalized Mean Bias (NMB)	$NMB = \frac{\sum_{i=1}^N (P_i - M_i)}{\sum_{i=1}^N M_i}$	%	−100 – ∞
Normalized Mean Error (NME)	$NME = \frac{\sum_{i=1}^N P_i - M_i }{\sum_{i=1}^N M_i}$	%	0 – ∞
Pearson correlation coefficient (r)	$r = \frac{(\sum_{i=1}^N P_i \cdot M_i - N \cdot \bar{P} \cdot \bar{M})}{(N-1) \cdot s_P \cdot s_M}$	Dimensionless	−1 – 1

^a P-AERIS results, M-AQMS results, N-number of cells of the domain, s-standard deviation of the dataset.

Table 6

Definition of the hypothetical scenario (HS) for additivity test.

SNAP code	Activity name	NO _x	
		VP _{HS} (%)	E _{HS} ^a
010101	Coal-fired power plants > 300 MW	20	282397
070101	Passenger cars-Highway driving	10	167737
070103	Passenger cars-Urban driving	50	164818
070303	HDV > 3.5 t-Urban driving	30	73695

^a Emissions are presented in annual metric tons (t yr⁻¹).

3.3. Definition of emission scenarios and projections

3.3.1. Hypothetical scenario for additivity test

The hypothetical emission scenario used for the additivity test (HS) consisted in a limited number of activity groups, whose emissions changed with respect to the BS according to Section 3.1 (Table 2). The VPs in every case were set arbitrarily and do not have any actual relevance because these were chosen to evaluate the model's response when high VPs are applied to the BS. To this respect, the term arbitrary refers to the fact that they were not calculated through the comparison of a projected (or future) emission against the baseline scenario (according to Section 2.2). The VPs and resulting emissions for this scenario (E_{HS}) are presented in Table 6.

3.3.2. Real emission scenario (2011)

The emission scenario of year 2011 (RS₁₁) was created to produce air quality estimates with AERIS that were further compared with observations. This was accomplished by using emission values of the 18 considered sectors (Table 2) reported by the Spanish and Portuguese Emission Inventories of the same year (Costa-Pereira et al., 2013; MAGRAMA, 2013) which consider decreases in emissions caused by the onset of the latest economic crisis in Europe. These values were introduced into AERIS in order to quantify the corresponding VPs of the relevant pollutants (NO_x, SO₂, PM₁₀, PM_{2.5}, NH₃, VOC) and subsequently run the model (Table 7). The direct estimation of these VPs was considered valid due to the consistency in emission-calculation methodologies between inventory versions (2007 and 2011). It should be noted that keeping chemical speciation profiles for NO_x, PM_{2.5} and VOC

constant in every simulation may not be true for future-year scenarios where important technological changes are expected in a particular sector. This may be the case of NO₂/NO_x ratios in the emissions from road traffic, which is an important factor for air quality levels in urban areas (Carslaw and Rhys-Tyler, 2013). This issue should be further investigated in the future but recent high-resolution modelling experiments in the Madrid metropolitan area, where emissions are strongly dominated by road traffic, (Borge et al., 2012) indicate that the errors brought about by this limitation may be relatively small for the purposes and spatial scale of AERIS.

3.3.3. Future emission scenario (2014)

The future scenario of emissions (RS₁₄) was developed to represent as accurately as possible the situation of emissions in year 2014 in Spain for NO_x, SO₂, PM₁₀, PM_{2.5}, NH₃ and VOC. The variations in each of the considered sectors are a consequence of the adoption of a set of feasible technical and non-technical measures on a national scale (Table 7). Most of these actions were derived from a combination of action plans and new legislation implemented between 2007 and 2014 by the National Government. Examples of these actions are the application of limits to fuel compositions, the introduction of more efficient combustion devices, the implementation of BATs, progressive changes to renewable energy sources, mobility and traffic restrictions in cities, etc. The RS₁₄ was elaborated with the SEP model and evaluated according to Lumbreras et al. (2008). The reason for the selection 2014 as case study is because it corresponds to the target year according to the local air quality plan (Madrid) for compliance with the limit values specified by Directive 2008/50/EC for NO₂. In a recent study, the possible compliance of the city of Madrid was analysed (Borge et al., 2014), for which a national projection scenario for 2014 (Spain) was elaborated.

It should be noted that RS₁₄ exhibits variations in the emissions of many more sectors (162 sectors) than those represented by the TMs of AERIS. However, we consider that the sectors simulated by AERIS are representative enough to provide a good picture of the air quality situation in the Iberian Peninsula. To this respect, the latest version of AERIS covers the following percentage of emissions of the BS: 75.8% for NO_x, 77.9% for SO₂, 89.5% for PM₁₀, 92.9% for PM_{2.5} and 90.4% for NH₃ (Table 2).

Table 7Variation percentages (VP) of the emission sectors considered for the 2011 (RS₁₁) and 2014 (RS₁₄) scenarios against the baseline scenario (BS)-2007.

SNAP code	Activity name	NO ₂		SO ₂		PM ₁₀		PM _{2.5}		NH ₃	
		VP ₂₀₁₁	VP ₂₀₁₄	VP ₂₀₁₁	VP ₂₀₁₄	VP ₂₀₁₁	VP ₂₀₁₄	VP ₂₀₁₁	VP ₂₀₁₄	VP ₂₀₁₁	VP ₂₀₁₄
010000	Coal-fired power plants >300 MW	-53.3	-58.8	-85.0	-88.2	-78.61	-74.9	-81.9	-78.9	-97.9	-100.0
020202	Residential plants <50 MW	-9.8	15.5	-32.3	-59.7	0.9	-5.7	0.7	-5.3	0.0	0.0
030000	Comb. in manufact.-area sources	-70.9	-58.8	-25.3	-33.0	-39.6	-53.0	-47.4	-57.3	0.0	0.0
040000	Production processes-area sources	-30.8	-4.3	-1.8	-7.3	-53.7	-0.8	-47.6	-2.3	-22.2	-35.8
070101	Passenger cars-Highway driving	-39.6	-62.1	-81.4	-80.9	-30.1	-48.1	-30.1	-48.1	-57.4	-35.0
070103	Passenger cars-Urban driving	-18.6	-17.3	-79.4	-75.1	-67.5	-67.5	-64.4	-67.5	244.3	114.8
070201	LDV < 3.5-Highway driving	-47.4	-47.7	-90.3	-87.0	-55.6	-68.3	-55.6	-68.3	-82.2	-56.0
070203	LDV < 3.5-Urban driving	-80.5	-83.2	-95.1	-93.7	-85.2	-90.1	-85.2	-90.1	-75.6	-46.0
070301	HDV >3.5 t-Highway driving	4.6	-3.9	-84.0	-80.7	-59.9	-69.1	-59.9	-69.1	-18.4	9.1
070303	HDV > 3.5 t-Urban driving	-55.7	-65.1	-93.81	-91.6	-85.1	-88.6	-85.1	-88.6	-67.8	-68.3
0707 + 08	Break, tire and road abrasion	0.0	0.0	0.0	0.0	-19.8	-17.5	-19.0	-16.7	0.0	0.0
080500	Airports LTO/yr > 10.000	-27.5	-27.5	-29.4	0.0	33.3	0.0	33.3	0.0	0.0	0.0
080600	Agriculture (machinery)	-47.3	-41.3	-40.2	-85.7	-90.6	-90.4	-90.6	-90.4	46.1	42.1
080800	Industry (machinery)	-67.3	-25.1	-85.2	105	-90.1	-42.3	-90.1	-50.5	0.0	33.8
100101	Cult. w/fertilizers-permanent crops	-66.6	-66.7	0.0	0.0	0.0	11.4	0.0	0.0	-4.8	-20.4
100102	Cult. w/fertilizers-arable crops	118.8	130.0	0.0	0.0	-15.5	0.0	0.0	0.0	5.4	-11.1
100500	Other agricultural activities	0.0	0.0	0.0	0.0	20.6	22.6	40.3	38.7	-5.8	-7.3
-	Other sources and sinks	5.3	12.8	172.5	11.4	-100.0	17.3	0.0	0.0	-96.5	-12.3
-	Portugal (total)	-24.4	0.0	-40.5	0.0	-13.7	0.0	-12.3	0.0	-4.6	0.0

For VOC: VP_{VOC2011} = -17.9%, VP_{VOC2014} = -22.4% (E_{VOC,BS} = 1,376,136 t yr⁻¹).

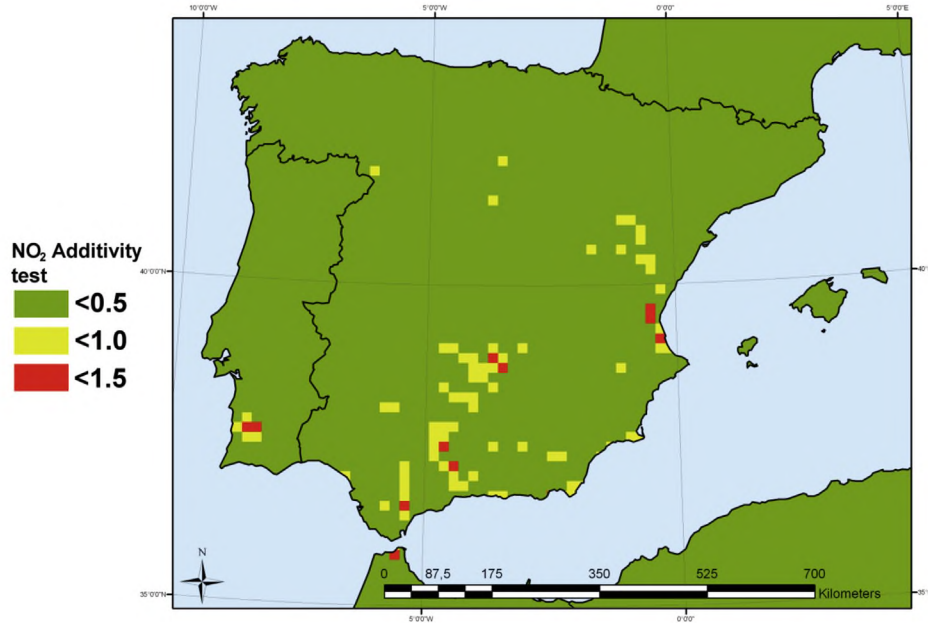


Fig. 4. Spatial performance of AERIS against the ordinary AQMS for the additivity test.

4. Results and discussion

4.1. Additivity test

The additivity test has revealed that for NO_2 , the modelling hypotheses implemented during the construction of AERIS seem reasonable. The main question here was assessing whether a TM on its own is able to reproduce a change in the pollutant concentration in the same way that this change is produced by the AQMS along with other varying sectors. The goal of the analysis is to gain insight on the flexibility of the modelling framework of AERIS.

Fig. 4 depicts the behaviour of the different cells of the domain for different thresholds of the additivity test. It can be seen that most cells (4416–98.1%) are below the lowest threshold, covering most of the modelling domain while a minority of cells are above $t = 1.0 \mu\text{g}/\text{m}^3$ and $t = 1.5 \mu\text{g}/\text{m}^3$ (73 and 11, 1.6% and 0.2% respectively). The spatial representation of this behaviour is relevant to detect the presence of problematic zones (i.e. hotspots) and to assure that the estimates are valid throughout the modelled domain. Domain-averaged results for the additivity test are presented in Table 8 for each of the evaluated sectors. As it can be seen, the resulting NO_2 mean annual concentrations calculated by both models are similar, with low mean absolute errors ($|X_{i,\text{AERIS}} - X_{i,\text{AQMS}}| < 0.5 \mu\text{g}/\text{m}^3$). Additionally, the normalized mean bias (NMB) for the complete domain equalled 4.1% and the normalized mean error 13.0% (NME), being both values below the $\text{NMB} \leq 15\%$ and $\text{NME} \leq 35\%$ limits for acceptable performance according to Boylan and Russell (2006). It should be noted that the estimates

produced by those cells in which $t = 1.5 \mu\text{g}/\text{m}^3$ are not to be discarded due to the fact that the general (domain-wide) performance is considered to be in range.

Despite the fact of having a limited number of sectors at the HS and only assessing one pollutant, the basic modelling approach implemented for AERIS seems adequate for representing either individual or group variations. It should be stressed out that this additivity test is able only to provide a rough estimate of the expected deviation between model estimates when different sectors change their emissions simultaneously and only for one pollutant (NO_2 in this case). Such a deviation is expected to grow and propagate as the number of sectors as well as the complexity of the evaluation increase.

4.2. General performance analysis of AERIS

The concentration fields provided by AERIS are presented as the most relevant indicators in terms of their significance with European-level policy: the 19th highest hourly concentration (NO_2), daylight AOT₄₀ (O_3), the annual mean concentration ($\text{PM}_{2.5}$) and the 25th highest daily concentration (SO_2). The spatial representation of these indicators is shown in Fig. 5. From a qualitative point of view, these concentration maps clearly identify pollution hotspots such as cities (i.e. Madrid, Barcelona) or large point-sources as a consequence of the implemented finer resolution of the modelled domain and the detailed emission inventories (when compared to European-level IAMs). For the concrete case of O_3 , high-concentration zones are evident in regions that are typically

Table 8

Results of the additivity test expressed as mean values for the entire domain.

Sector	Activity name	$X_{i,\text{AERIS}} (\mu\text{g}/\text{m}^3)^a$	$X_{i,\text{AQMS}} (\mu\text{g}/\text{m}^3)$	$ X_{i,\text{AERIS}} - X_{i,\text{AQMS}} $
010101 (S)	Coal-fired power plants > 300 MW	4.41	4.67	0.27
070101 (S)	Passenger cars-Highway driving	4.42	4.41	0.05
070103 (S)	Passenger cars-Urban driving	4.48	4.51	0.14
070303 (S)	HDV > 3.5 t-Urban driving	4.43	4.44	0.01
$\sum_i S_i$		—	—	0.48
All sectors (HS)		4.62	4.88	0.26

^a X-is either S (sector) or HS (hypothetic scenario).

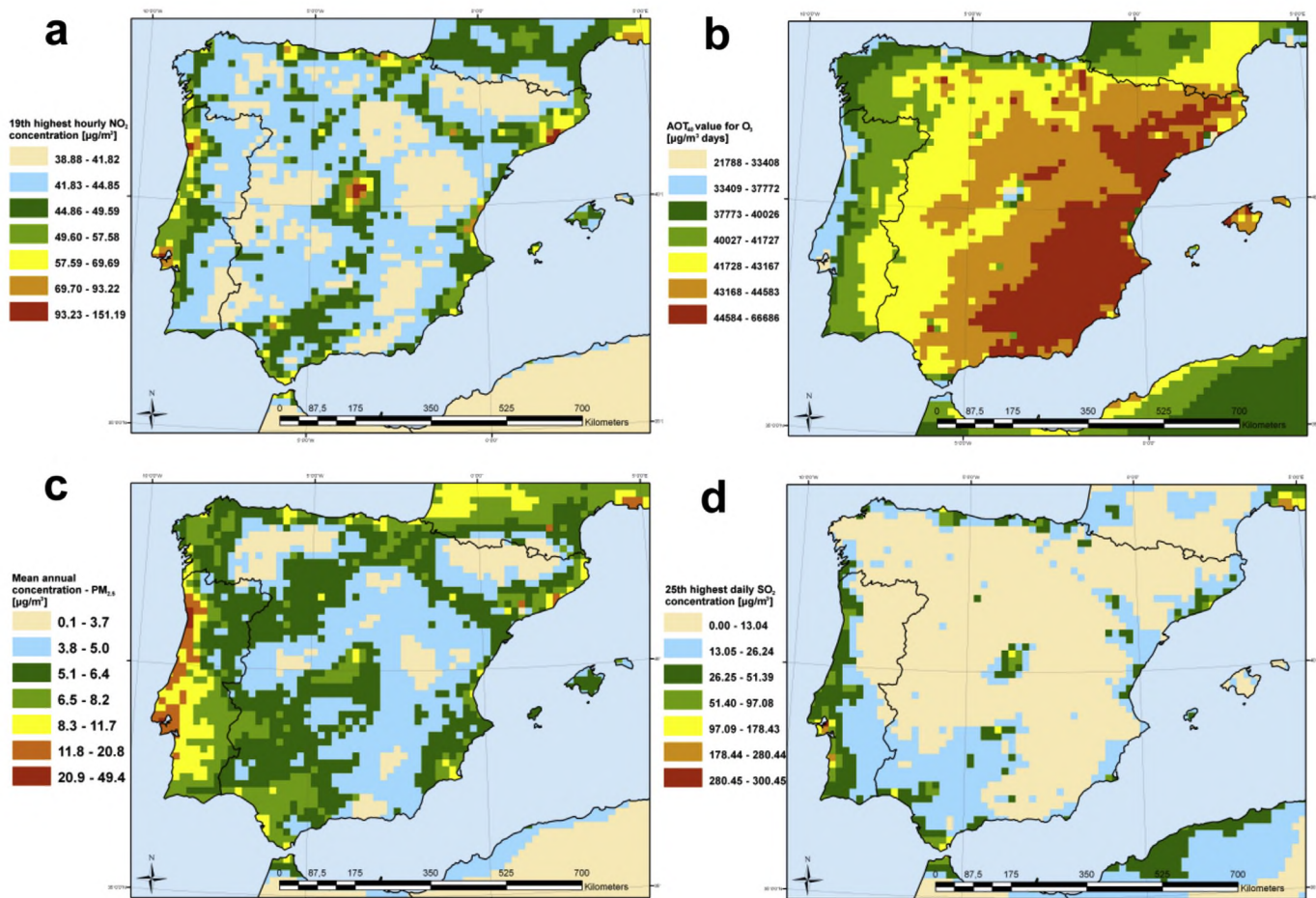


Fig. 5. Concentration results of the real policy scenario (2014) a) 19th highest hourly concentration- NO_2 [$\mu\text{g}/\text{m}^3$] b) daylight $\text{AOT}_{40-\text{O}_3}$ [$\mu\text{g}/\text{m}^3\text{h}$] c) annual mean concentration- $\text{PM}_{2.5}$ [$\mu\text{g}/\text{m}^3$] d) 25th highest hourly concentration- SO_2 [$\mu\text{g}/\text{m}^3$].

affected by summer events such as the Mediterranean coast of Spain (de Andrés et al., 2012). The fact of presenting concentrations using these indicators is useful for assessing whether some specific locations might attain European and National legislation limits for future emission scenarios. Moreover, these indicators can be easily related with impacts or exposure levels and are certainly useful for the future construction of health and ecosystems-related modules.

4.2.1. Validation of AERIS against AQMS

The statistical comparison of the AERIS estimates and the AQMS outputs by the means of benchmarking indicators is shown in Table 9. The estimates provided for NO_2 are characterized by slight tendencies towards overprediction as evidenced by the MB and the NMB values, while the total error (ME) roughly reaches $0.35 \mu\text{g}/\text{m}^3$. However, the accuracy of NO_2 -predictions might be slightly compromised since $\text{NMB} = 19.82\%$ indicates overprediction (being

above the recommended threshold of $|\text{NMB}| \leq 15\%$) (Russell and Dennis, 2000). A similar behaviour is observed for SO_2 , where the same tendencies exist but with a lower error presence ($\text{NME} = 17.14\%$). The overpredictive character of AERIS for these pollutants, whose TMs do not account for the totality of emission sectors present in the RS_{14} , might be explained by the loss of accuracy that is inherent to any statistical parameterization and the fact that the emission reductions might be concentrated in those sectors for which the IAM has considered a TM.

For the rest of pollutants, the opposite behaviour was witnessed. For instance, $\text{PM}_{2.5}$ shows a general underpredictive trend, which is also the highest among the studied species ($\text{NMB} = -5.39\%$). This deficit in $\text{PM}_{2.5}$ predictions might be explained by the fact that not all the emission sectors are actually simulated by AERIS. The parameterization of the secondary component of $\text{PM}_{2.5}$ might also be a cause of this behaviour. Additionally, the O_3 estimates were calculated by an additional parameterization that depends on the NO_2 TMs so an additional component for statistical mismatch is to be expected for this pollutant. In every case, the Pearson correlation coefficients (Fig. 6) are way above the performance thresholds of $r = 0.65$ for gaseous pollutants and $r = 0.40$ for particulate matter defined by Thunis et al. (2011), which reveal a good correspondence between models. A small accumulation of error between models was also observed, as the NME for all pollutants lied below the recommended values of performance ($\text{NME} \leq 35\%$ for gases and $\text{NME} \leq 50\%$ for particles) (USEPA, 2007; Chemel et al., 2010).

Table 9
Statistic indicators of comparison between AERIS and the conventional AQMS for RS_{14} .

Pollutant	MB ($\mu\text{g}/\text{m}^3$)	ME ($\mu\text{g}/\text{m}^3$)	NMB (%)	NME (%)	r	FAC2 (%)
NO_2	0.32	0.35	19.82	21.96	0.9787	99.7
SO_2	0.32	0.47	11.49	17.14	0.9806	93.9
$\text{PM}_{2.5}$	-0.34	0.43	-5.39	6.81	0.9891	100.0
NH_3	-0.02	0.06	-4.35	10.38	0.9851	100.0
O_3	-0.26	-0.76	-0.27	0.78	0.9706	100.0

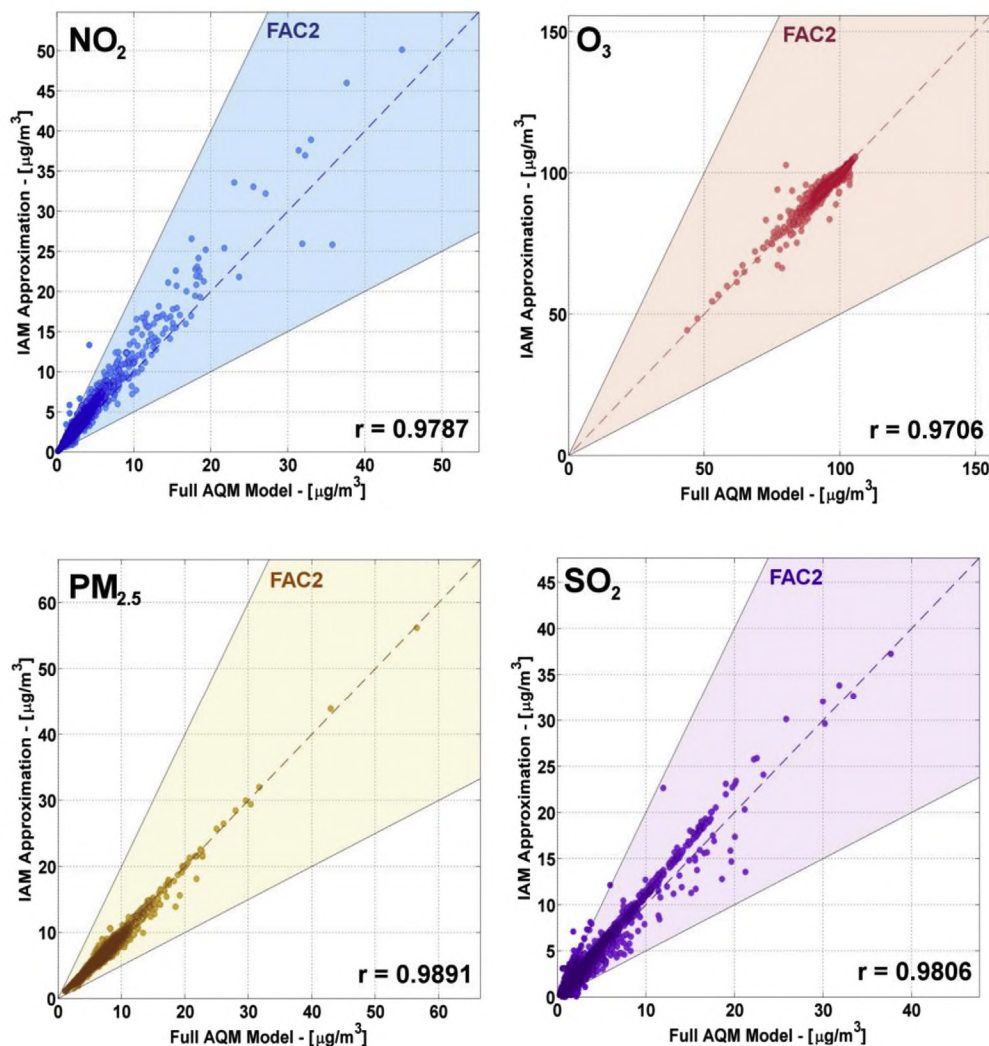


Fig. 6. Comparison of the mean annual concentration calculated with AERIS and the full AQMS for the 2014 real policy scenario (RS₁₄). Comparison units for NO₂, PM_{2.5}, SO₂: $\mu\text{g}/\text{m}^3$, O₃: $\mu\text{g}/\text{m}^3\text{h}$.

4.2.2. Validation of AERIS against observations

In general, the correspondence of AERIS with air quality observations from the selected network (Table 10) is adequate, according to the considered model validation criteria (Thunis et al., 2011). Special attention needs to be put on the statistical metrics for PM_{2.5} since only four monitoring stations were used (Portugal). Although the correspondence between datasets is the best among the analysed pollutants, any interpretations on model-skills for PM_{2.5} need to be put into perspective. In every other case, the Pearson correlation coefficient (r) is above $r = 0.65$ which hints on the linear correspondence between values (Fig. 7). Additionally, one can see that AERIS has a tendency for overpredicting air quality levels from the fact that the MB and NMB values for every pollutant are

positive, of which only NO₂ is in range ($|\text{NMB}| \leq 15\%$) (Boylan and Russell, 2006).

This fact is especially evident for SO₂, (NMB = 77.8%, FAC2 = 58%) indicating that the TMs might not be able to catch all the effective reductions in emissions that took place between 2007 (BS) and 2011. An example of this could be the substitution of coal for other fuels by some coal-power plants in northern Spain as a consequence of the introduction of fuel composition limits immediately after 2007. In the same line, an additional explanation for this deviation could be the fact that SO₂ greatly depends on local sources and environmental factors (i.e. emissions from industries) (Chemel et al., 2010). In the case of O₃, the slighter overpredictive character is observed although the value of NME (24.9%) lies below the NME $\leq 35\%$ model performance threshold (Russell and Dennis, 2000). To this respect, the parent-AQMS of AERIS (the SERCA project) exhibits some bias towards overprediction for ozone, as shown in de Andr  s et al. (2012).

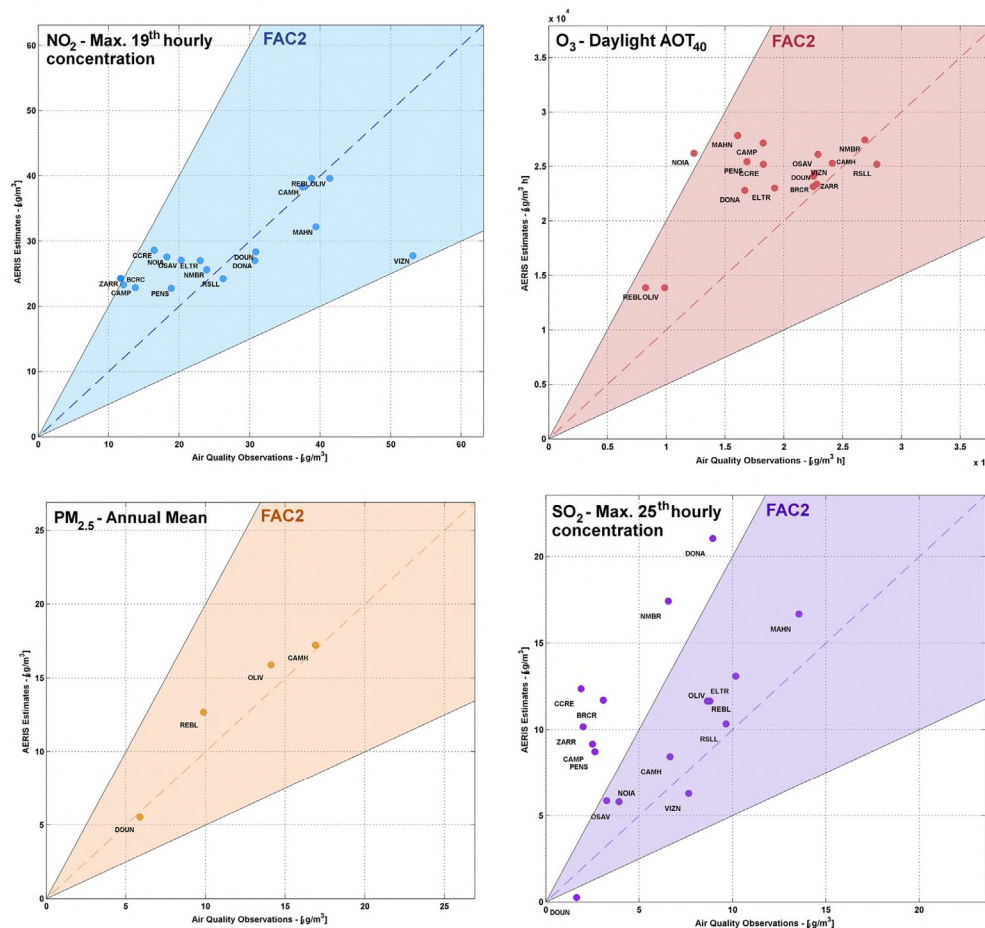
It is worth noting that the number of chosen monitoring locations is limited, due to the fact that a geographically well-distributed network of rural background stations was preferred in order to have observations that might not be influenced by local gradients and that would be representative of the 16 km-scale of AERIS. In general, another issue that needs to be kept in mind is the

Table 10

Statistic indicators of comparison between AERIS and observations for RS₁₁.

Pollutant	MB ^a	ME ^a	NMB (%)	NME (%)	r	FAC2 (%)
NO ₂ (Max 19th)	1.75	6.75	6.52	25.18	0.8163	94.1
O ₃ (AOT ₄₀)	4489	4808	23.27	24.92	0.7852	94.1
PM _{2.5} (Ann. Mean)	0.27	0.31	9.82	11.25	0.9973	100.0
SO ₂ (Max 25th)	4.64	4.97	77.84	83.27	0.7432	58.8

^a Units of MB/ME for NO₂, PM_{2.5}, SO₂: $\mu\text{g}/\text{m}^3$, O₃: $\mu\text{g}/\text{m}^3\text{h}$.



fact that TMs were built using meteorological fields from year 2007 so a deviation between model predictions and observations was to be expected. Despite the fact that 2011 was not considered atypical in the meteorological sense (AEMET, 2012), any conclusions drawn from a direct comparison with observations should be handled with care.

At this point it is worth noting that the use of AERIS is an advantage when used in screening activities, due to the fact that it avoids incurring in long computing times while showing similarities in result performance when compared to the conventional AQMS. For example, simulating one year with AERIS, on a 2.0 GHz (1GB_{RAM}) Athlon™ 64 processor, takes about 1.5s of CPU-time. On the other hand, running an annual simulation of the AQMS needs approximately 168 h of CPU-time using a 16-node computer cluster with a 3.3 GHz IntelDuo™ microprocessor each. Furthermore, AERIS can be easily used in any Windows™-PC provided that MATLAB® is installed first, while it is well-known that a high degree of technical and computing expertise is needed for configuring and running an AQMS, as well as for processing the obtained results.

The construction of AERIS as an IAM intended to evaluate the effect of policies directed to tackle the air pollution problem is an improvement in the current availability of modelling resources for stakeholders in Spain. The parameterization of a fully contrasted and operative AQMS (WRF-SMOKE-CMAQ) proved to be consistent enough to make the results yielded by AERIS reasonable and realistic, according to the results presented in this paper. In general terms considering a scale finer than the European-level (i.e. GAINS) for the description of the Iberian Peninsula allowed us to obtain outputs with a higher detail degree. A reasonable level of reproduction of the outputs yielded by the AQMS has been witnessed, showing a slight tendency for overprediction but always within good-performance ranges defined in scientific literature. In a similar line, AERIS presented a moderate level of statistic correspondence with air quality observations from representative monitoring locations. These analyses revealed that the limitations of AERIS lie precisely on the fact that it constitutes a general parameterization of an AQMS and its ancillary data, which are very likely to change as emission scenarios are changed with respect of the considered baseline scenario. As a consequence, stakeholders should be fully aware about the limitations associated with AERIS when destined to policy-support activities.

scenarios. When addressing the “fitness-for-purpose” of AERIS, it should be noted that it has been created under a policy-driven framework and by no means should be considered as a substitute of the ordinary AQMS. To this respect, the clear advantages it has in software requirements, configuration and running practices as well as CPU-time should be contrasted against the saliency and credibility of the estimates it produces. Moreover, an effort in reconciling the complexity of modelling with the conciseness of policies was made, which is reflected in the conceptual and computational structures of AERIS. It can be anticipated that the results provided by this IAM will help to gain further insight on the general situation of air quality in Spain and Europe as advanced by the validation practices addressed on this paper. Additionally, it should be reminded that AERIS is an IAM currently under development to include the quantification of impacts to ecosystems, human health and control costs. Improvements on issues such as the consideration of constant speciation profiles or a single-year meteorology will be undertaken as part of the usual model evaluation framework.

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